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Chemical Equilibria in Chlorination of Clay

By A. D. Mah

UNITED STATES DEPARTMENT OF THE INTERIOR

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UNITED STATES DEPARTMENT OF THE INTERIOR
James G. Watt, Secretary

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Robert C. Horton, Director

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CHEMICAL EQUILIBRIA IN CHLORINATION OF CLAY

By A. D. Mah[1]

ABSTRACT

To assist Bureau of Mines research in extractive metallurgy and to add to the thermodynamic data base useful to others, energy calculations were made for 63 reactions relating to investigations on the production of anhydrous aluminum chloride from chlorination of clay.

INTRODUCTION

As part of a continuing effort to obtain efficient and environmentally acceptable utilization of natural resources, the Bureau of Mines is conducting research on the economical recovery of aluminum from domestic clay. To aid research and guide the direction of investigations, energy calculations were made for reactions relating to the chlorination-reduction of clay and the purification and recovery of anhydrous aluminum chloride.

The values of thermodynamic properties of compounds employed in these calculations were generally taken from critical compilations such as those by Kelley (2-4),[2] the National Bureau of Standards (5), and Wagman (6), and from selected original sources. No high-temperature enthalpy data were available for clay. Since clay dehydrates readily at moderate temperatures prior to chlorination, and, as a practical matter, water must be absent during chlorination, the combination of 1 mole Al_2O_3 plus 2 moles SiO_2 was used to represent dehydrated clay in these reactions. This representation is indicated by the use of brackets in the equations. Other needed properties not available in the literature were estimated.

Sixty-three reactions for which thermodynamic data were critically evaluated and compiled, are listed in the "Contents," as well as in the "Directory of Reactions." The standard enthalpy change of reaction, standard Gibbs energy change of reaction, and logarithm of the equilibrium constant of reaction as functions of temperature are given in correspondingly numbered tables. The abbreviations used in the table headings and equations are as follows:

T = Temperature in kelvins
K = Kelvin, the unit of temperature

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[1]Research chemist, Albany Research Center, Bureau of Mines, Albany, Oreg.

[2]Underlined numbers in parentheses refer to items in the list of references at the end of this report.

ΔH° = Standard enthalpy change of reaction
ΔG° = Standard Gibbs energy change of reaction
log K = Base 10 logarithm of the equilibrium constant of reaction
(s) = Solid
(ℓ) = Liquid
(g) = Gas

DIRECTORY OF REACTIONS
(In alphabetical sequence of first element in first reactant)

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NOTE: Stable forms of C and Al_2O_3 are graphite and alpha-alumina, respectively.

TABLE 1. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$[Al_2O_3(s) + 2SiO_2(s)] + 7Cl_2(g) + 3.5C(s) = Al_2Cl_6(g) + 2SiCl_4(g) + 3.5CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-116.9	-129.0	94.56	900	-118.3	-154.1	37.42
300	-116.9	-129.1	94.05	1000	-118.8	-158.1	34.55
400	-116.3	-133.2	72.78	1100	-119.3	-162.0	32.19
500	-116.2	-137.5	60.10	1200	-119.8	-165.8	30.20
600	-116.3	-141.7	51.61	1300	-120.3	-169.6	28.51
700	-116.6	-145.9	45.55	1400	-120.8	-173.4	27.07
800	-117.2	-150.1	41.01	1500	-121.4	-177.1	25.80
[1]847	-117.7	-152.0	39.22	1600	-122.0	-180.8	24.70
847	-118.0	-152.0	39.22	1700	-122.5	-184.5	23.72

[1]Transition point of SiO_2.

TABLE 2. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$[Al_2O_3(s) + 2SiO_2(s)] + 7Cl_2(g) + 3.5C(s) = 2AlCl_3(g) + 2SiCl_4(g) + 3.5CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-86.1	-109.1	79.97	900	-89.8	-154.8	37.59
300	-86.1	-109.2	79.55	1000	-90.7	-162.0	35.41
400	-85.9	-117.0	63.93	1100	-91.6	-169.1	33.60
500	-86.1	-124.8	54.55	1200	-92.5	-176.0	32.05
600	-86.6	-132.4	48.23	1300	-93.4	-183.0	30.77
700	-87.4	-140.0	43.71	1400	-94.3	-189.8	29.63
800	-88.3	-147.5	40.30	1500	-95.3	-196.6	28.64
[1]847	-89.0	-150.9	38.94	1600	-96.2	-203.3	27.77
847	-89.3	-150.9	38.94	1700	-97.2	-210.0	27.00

[1]Transition point of SiO_2.

TABLE 3. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$[Al_2O_3(s) + 2SiO_2(s)] + 7Cl_2(g) + 7C(s) = Al_2Cl_6(g) + 2SiCl_4(g) + 7CO(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	27.4	-28.5	20.89	900	25.2	-143.2	34.77
300	27.4	-28.9	21.05	1000	23.9	-161.9	35.38
400	28.7	-47.9	26.17	1100	22.6	-180.4	35.84
500	29.1	-67.1	29.33	1200	21.2	-198.8	36.21
600	28.8	-86.3	31.43	1300	19.8	-217.1	36.50
700	28.1	-105.4	32.91	1400	18.3	-235.2	36.72
800	26.9	-124.4	33.98	1500	16.8	-253.3	36.91
[1]847	26.2	-133.3	34.40	1600	15.2	-271.2	37.04
847	25.8	-133.3	34.40	1700	13.7	-289.1	37.17

[1]Transition point of SiO_2.

TABLE 4. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$[Al_2O_3(s) + 2SiO_2(s)] + 7Cl_2(g) + 7C(s) = 2AlCl_3(g) + 2SiCl_4(g) + 7CO(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	58.2	-8.7	6.38	900	53.7	-143.9	34.94
300	58.2	-9.1	6.63	1000	52.0	-165.8	36.24
400	59.1	-31.6	17.27	1100	50.3	-187.5	37.25
500	59.1	-54.4	23.78	1200	48.6	-209.0	38.06
600	58.5	-77.0	28.05	1300	46.7	-230.4	38.73
700	57.4	-99.5	31.07	1400	44.9	-251.7	39.29
800	55.8	-121.8	33.27	1500	42.9	-272.8	39.75
[1]847	54.9	-132.2	34.11	1600	41.0	-293.7	40.12
847	54.5	-132.2	34.11	1700	39.0	-314.6	40.44

[1]Transition point of SiO_2.

TABLE 5. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$[Al_2O_3(s) + 2SiO_2(s)] + 7Cl_2(g) + 7CO(g) = Al_2Cl_6(g) + 2SiCl_4(g) + 7CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-261.2	-229.4	168.15	900	-261.8	-165.0	40.07
300	-261.2	-229.2	166.97	1000	-261.5	-154.2	33.70
400	-261.3	-218.6	119.44	1100	-261.2	-143.5	28.51
500	-261.4	-207.8	90.83	1200	-260.8	-132.9	24.20
600	-261.4	-197.1	71.79	1300	-260.4	-122.2	20.54
700	-261.4	-186.4	58.20	1400	-260.0	-111.6	17.42
800	-261.4	-175.7	48.00	1500	-259.6	-101.0	14.72
[1]847	-261.5	-170.7	44.05	1600	-259.2	-90.5	12.36
847	-261.9	-170.7	44.05	1700	-258.8	-79.9	10.27

[1]Transition point of SiO_2.

TABLE 6. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$[Al_2O_3(s) + 2SiO_2(s)] + 7Cl_2(g) + 7CO(g) = 2AlCl_3(g) + 2SiCl_4(g) + 7CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-230.4	-209.5	153.57	900	-233.3	-165.6	40.21
300	-230.4	-209.4	152.55	1000	-233.4	-158.1	34.55
400	-230.9	-202.3	110.53	1100	-233.5	-150.6	29.92
500	-231.3	-195.1	85.28	1200	-233.5	-143.1	26.06
600	-231.7	-187.9	68.44	1300	-233.5	-135.5	22.78
700	-232.1	-180.5	56.35	1400	-233.5	-128.0	19.98
800	-232.5	-173.1	47.29	1500	-233.5	-120.5	17.56
[1]847	-232.8	-169.6	43.76	1600	-233.4	-113.0	15.44
847	-233.2	-169.6	43.76	1700	-233.4	-105.4	13.55

[1]Transition point of SiO_2.

TABLE 7. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Al_2O_3(s) + 3Cl_2(g) + 1.5C(s) = Al_2Cl_6(g) + 1.5CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-52.3	-52.3	∞	1000	-50.2	-67.1	14.66
100	-51.8	-52.4	114.52	1100	-50.4	-68.8	13.67
200	-50.8	-53.5	58.46	1200	-50.6	-70.5	12.84
298.15	-50.2	-55.0	40.32	1300	-50.8	-72.1	12.12
300	-50.2	-55.0	40.07	1400	-51.1	-73.7	11.51
400	-49.8	-56.7	30.98	1500	-51.4	-75.3	10.97
500	-49.7	-58.4	25.53	1600	-51.7	-76.9	10.50
600	-49.7	-60.2	21.93	1700	-52.0	-78.5	10.09
700	-49.7	-61.9	19.33	1800	-52.4	-80.0	9.71
800	-49.8	-63.7	17.40	1900	-52.7	-81.6	9.39
900	-50.0	-65.4	15.88	2000	-53.1	-83.1	9.08

TABLE 8. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Al_2O_3(s) + 3Cl_2(g) + 1.5C(s) = 2AlCl_3(g) + 1.5CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-21.3	-21.3	∞	1000	-22.1	-71.0	15.52
100	-20.5	-25.1	54.86	1100	-22.6	-75.9	15.08
200	-19.7	-30.0	32.78	1200	-23.3	-80.7	14.70
298.15	-19.4	-35.1	25.73	1300	-23.9	-85.4	14.36
300	-19.4	-35.2	25.64	1400	-24.6	-90.2	14.08
400	-19.4	-40.5	22.13	1500	-25.3	-94.8	13.81
500	-19.6	-45.7	19.98	1600	-26.0	-99.4	13.58
600	-20.0	-50.9	18.54	1700	-26.7	-104.0	13.37
700	-20.4	-56.0	17.48	1800	-27.4	-108.5	13.17
800	-20.9	-61.1	16.69	1900	-28.2	-113.0	13.00
900	-21.5	-66.1	16.05	2000	-28.9	-117.5	12.84

TABLE 9. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$SiO_2(s) + 2Cl_2(g) + C(s) = SiCl_4(g) + CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-33.4	-37.0	27.12	900	-34.2	-44.3	10.76
300	-33.4	-37.0	26.95	1000	-34.3	-45.5	9.94
400	-33.3	-38.3	20.93	1100	-34.5	-46.6	9.26
500	-33.2	-39.5	17.27	1200	-34.6	-47.7	8.69
600	-33.3	-40.8	14.86	1300	-34.7	-48.8	8.20
700	-33.5	-42.0	13.11	1400	-34.9	-49.8	7.77
800	-33.7	-43.2	11.80	1500	-35.0	-50.9	7.42
[1]847	-33.9	-43.7	11.28	1600	-35.1	-52.0	7.10
847	-34.1	-43.7	11.28	1700	-35.3	-53.0	6.81

[1] Transition point of SiO_2.

TABLE 10. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$TiO_2(s) + 2Cl_2(g) + C(s) = TiCl_4(g) + CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-50.8	-55.5	40.68	1200	-52.5	-68.8	12.53
300	-50.8	-55.5	40.43	1300	-52.7	-70.2	11.80
400	-50.8	-57.1	31.20	1400	-53.0	-71.5	11.16
500	-50.9	-58.7	25.66	1500	-53.2	-72.9	10.62
600	-51.1	-60.2	21.93	1600	-53.5	-74.1	10.12
700	-51.3	-61.7	19.26	1700	-53.8	-75.4	9.69
800	-51.6	-63.2	17.27	1800	-54.1	-76.7	9.31
900	-51.8	-64.7	15.71	1900	-54.5	-77.9	8.96
1000	-52.0	-66.1	14.45	2000	-54.8	-79.2	8.65
1100	-52.3	-67.5	13.41				

TABLE 11. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Fe_2O_3(s) + 3Cl_2(g) + 1.5C(s) = Fe_2Cl_6(g) + 1.5CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-102.9	-102.9	∞	[1] 960	-104.8	-120.6	27.46
100	-102.2	-103.4	225.98	1000	-105.0	-121.3	26.51
200	-101.1	-105.1	114.85	1100	-105.6	-122.9	24.42
298.15	-100.6	-107.2	78.58	1200	-106.1	-124.4	22.66
300	-100.6	-107.2	78.10	1300	-106.6	-125.9	21.17
400	-100.5	-109.4	59.77	1400	-107.2	-127.4	19.89
500	-100.8	-111.7	48.82	1500	-107.7	-128.8	18.77
600	-101.2	-113.8	41.45	1600	-108.2	-130.2	17.78
700	-101.9	-115.8	36.15	1700	-108.7	-131.6	16.92
800	-102.7	-117.8	32.18	1800	-109.2	-132.9	16.14
900	-103.8	-119.6	29.04				

[1]Curie temperature of Fe_2O_3.

TABLE 12. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Fe_2O_3(s) + 3Cl_2(g) + 1.5C(s) = 2FeCl_3(g) + 1.5CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-66.9	-66.9	∞	[1]960	-72.4	-118.3	26.93
100	-66.2	-71.5	156.26	1000	-72.8	-120.2	26.27
200	-65.5	-77.1	84.25	1100	-73.7	-124.9	24.82
298.15	-65.5	-82.9	60.77	1200	-74.7	-129.5	23.59
300	-65.5	-83.0	60.47	1300	-75.6	-134.0	22.53
400	-65.9	-88.7	48.46	1400	-76.6	-138.5	21.62
500	-66.5	-94.4	41.26	1500	-77.5	-142.9	20.82
600	-67.4	-99.9	36.39	1600	-78.4	-147.2	20.11
700	-68.5	-105.2	32.84	1700	-79.3	-151.4	19.46
800	-69.7	-110.4	30.16	1800	-80.2	-155.7	18.90
900	-71.2	-115.4	28.02				

[1]Curie temperature of Fe_2O_3.

TABLE 13. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$CaO(s) + Cl_2(g) + 0.5C(s) = CaCl_2(s,\ell) + 0.5CO_2(g)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-85.4	-81.7	59.89	1045	-77.2	-73.4	15.35
300	-85.4	-81.7	59.52	1100	-76.8	-73.2	14.54
400	-85.2	-80.5	43.98	1200	-76.2	-73.0	13.30
500	-85.0	-79.3	34.66	1300	-75.5	-72.7	12.22
600	-84.9	-78.2	28.48	1400	-74.9	-72.5	11.32
700	-84.7	-77.1	24.07	1500	-74.3	-72.4	10.55
800	-84.6	-76.0	20.76	1600	-73.6	-72.3	9.88
900	-84.4	-74.9	18.19	1700	-73.0	-72.2	9.28
1000	-84.1	-73.9	16.15	1800	-72.4	-72.2	8.77
[1]1045	-84.0	-73.4	15.35				

[1]Melting point of $CaCl_2$.

TABLE 14. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$Na_2O(s) + Cl_2(g) + 0.5C(s) = 2NaCl(s,\ell) + 0.5CO_2(g)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-143.9	-140.3	102.84	900	-142.3	-134.1	32.56
300	-143.9	-140.3	102.21	1000	-141.9	-133.2	29.11
400	-143.6	-139.1	76.00	[1]1073.8	-141.7	-132.6	26.99
500	-143.3	-138.0	60.32	1073.8	-128.2	-132.6	26.99
600	-143.1	-137.0	49.90	1100	-128.1	-132.7	26.37
700	-142.9	-136.0	42.46	1200	-128.0	-133.1	24.24
800	-142.6	-135.0	36.88	1300	-128.5	-133.5	22.44

[1]Melting point of NaCl.

TABLE 15. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$K_2O(s) + Cl_2(g) + 0.5C(s) = 2KCl(s,\ell) + 0.5CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-169.4	-165.9	121.61	900	-168.3	-159.4	38.71
300	-169.4	-165.8	120.79	1000	-167.8	-158.4	34.62
400	-169.2	-164.7	89.99	[1]1045	-167.6	-158.0	33.04
500	-169.1	-163.6	71.51	1045	-155.1	-158.0	33.04
600	-168.9	-162.5	59.19	1100	-154.6	-158.1	31.41
700	-168.7	-161.4	50.39	[2]1154	-154.2	-158.3	29.98
800	-168.5	-160.4	43.82				

[1]Melting point of KCl.
[2]Decomposition point of K_2O.

TABLE 16. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Al_2O_3(s) + 3Cl_2(g) + 3C(s) = Al_2Cl_6(g) + 3CO(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	7.1	7.1	∞	1000	11.0	-68.8	15.04
100	8.6	2.5	-5.46	1100	10.4	-76.7	15.24
200	10.4	-4.4	4.81	1200	9.8	-84.6	15.41
298.15	11.6	-11.9	8.72	1300	9.2	-92.4	15.53
300	11.7	-12.1	8.81	1400	8.5	-100.2	15.64
400	12.3	-20.1	10.98	1500	7.8	-108.0	15.74
500	12.6	-28.3	12.37	1600	7.1	-115.7	15.80
600	12.5	-36.4	13.26	1700	6.3	-123.3	15.85
700	12.3	-44.6	13.92	1800	5.6	-130.9	15.89
800	11.9	-52.7	14.40	1900	4.8	-138.5	15.93
900	11.5	-60.8	14.76	2000	4.0	-146.0	15.95

TABLE 17. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Al_2O_3(s) + 3Cl_2(g) + 3C(s) = 2AlCl_3(g) + 3CO(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	38.0	38.0	∞	1000	39.1	-72.7	15.89
100	39.8	29.8	-65.13	1100	38.2	-83.8	16.65
200	41.5	19.1	-20.87	1200	37.2	-94.8	17.27
298.15	42.4	7.9	-5.79	1300	36.1	-105.8	17.79
300	42.5	7.7	-5.61	1400	35.1	-116.7	18.22
400	42.8	-3.9	2.13	1500	34.0	-127.5	18.58
500	42.6	-15.6	6.82	1600	32.8	-138.2	18.88
600	42.2	-27.2	9.91	1700	31.7	-148.8	19.13
700	41.6	-38.7	12.08	1800	30.5	-159.4	19.35
800	40.8	-50.1	13.69	1900	29.3	-169.9	19.54
900	40.0	-61.4	14.91	2000	28.1	-180.4	19.71

TABLE 18. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$SiO_2(s) + 2Cl_2(g) + 2C(s) = SiCl_4(g) + 2CO(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	7.9	-8.3	6.08	900	6.8	-41.2	10.00
300	7.9	-8.4	6.12	1000	6.5	-46.6	10.18
400	8.2	-13.9	7.59	1100	6.1	-51.9	10.31
500	8.3	-19.4	8.48	1200	5.7	-57.1	10.40
600	8.1	-24.9	9.07	1300	5.3	-62.3	10.47
700	7.9	-30.4	9.49	1400	4.9	-67.5	10.54
800	7.5	-35.9	9.81	1500	4.5	-72.7	10.59
[1]847	7.2	-38.4	9.91	1600	4.1	-77.8	10.63
847	7.0	-38.4	9.91	1700	3.7	-82.9	10.66

[1]Transition point of SiO_2.

TABLE 19. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$TiO_2(s) + 2Cl_2(g) + 2C(s) = TiCl_4(g) + 2CO(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-9.6	-26.8	19.64	1200	-12.2	-78.3	14.26
300	-9.6	-26.9	19.60	1300	-12.7	-83.8	14.09
400	-9.4	-32.7	17.87	1400	-13.2	-89.2	13.92
500	-9.4	-38.6	16.87	1500	-13.8	-94.6	13.78
600	-9.6	-44.4	16.17	1600	-14.3	-100.0	13.66
700	-10.0	-50.2	15.67	1700	-14.9	-105.3	13.54
800	-10.4	-55.9	15.27	1800	-15.5	-110.6	13.43
900	-10.8	-61.6	14.96	1900	-16.1	-115.9	13.33
1000	-11.3	-67.2	14.69	2000	-16.8	-121.1	13.23
1100	-11.7	-72.7	14.44				

TABLE 20. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Fe_2O_3(s) + 3Cl_2(g) + 3C(s) = Fe_2Cl_6(g) + 3CO(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-43.6	-43.6	∞	[1]960	-43.5	-119.7	27.25
100	-41.8	-48.5	106.00	1000	-43.8	-122.9	26.86
200	-39.8	-56.0	61.19	1100	-44.7	-130.8	25.99
298.15	-38.3	-64.1	46.99	1200	-45.7	-138.5	25.22
300	-38.7	-64.3	46.84	1300	-46.6	-146.2	24.58
400	-38.4	-72.9	39.83	1400	-47.5	-153.9	24.02
500	-38.5	-81.5	35.62	1500	-48.5	-161.5	23.53
600	-39.1	-90.0	32.78	1600	-49.4	-168.9	23.07
700	-39.9	-98.5	30.75	1700	-50.3	-176.4	22.68
800	-40.9	-106.8	29.18	1800	-51.3	-183.8	22.32
900	-42.3	-114.9	27.90				

[1]Curie temperature of Fe_2O_3.

TABLE 21. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Fe_2O_3(s) + 3Cl_2(g) + 3C(s) = 2FeCl_3(g) + 3CO(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-7.5	-7.5	∞	[1]960	-11.1	-117.4	26.73
100	-5.8	-16.6	36.28	1000	-11.6	-121.8	26.62
200	-4.3	-28.0	30.60	1100	-12.9	-132.8	26.38
298.15	-3.7	-39.8	29.17	1200	-14.2	-143.6	26.15
300	-3.6	-40.0	29.14	1300	-15.6	-154.3	25.94
400	-3.7	-52.2	28.52	1400	-16.9	-165.0	25.76
500	-4.3	-64.2	28.06	1500	-18.2	-175.5	25.57
600	-5.2	-76.1	27.72	1600	-19.6	-185.9	25.39
700	-6.4	-87.8	27.41	1700	-20.9	-196.3	25.24
800	-7.9	-99.4	27.15	1800	-22.3	-206.6	25.08
900	-9.7	-110.7	26.88				

[1]Curie temperature of Fe_2O_3.

TABLE 22. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$CaO(s) + Cl_2(g) + C(s) = CaCl_2(s,\ell) + CO(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-64.8	-67.3	49.33	1045	-56.8	-74.9	15.66
300	-64.8	-67.4	49.10	1100	-56.5	-75.9	15.08
400	-64.5	-68.3	37.32	1200	-56.0	-77.7	14.15
500	-64.3	-69.2	30.25	1300	-55.5	-79.5	13.37
600	-64.1	-70.3	25.61	1400	-55.0	-81.4	12.71
700	-64.0	-71.3	22.26	1500	-54.5	-83.3	12.14
800	-64.0	-72.3	19.75	1600	-54.0	-85.2	11.64
900	-63.9	-73.4	17.82	1700	-53.6	-87.1	11.20
1000	-63.7	-74.4	16.26	1800	-53.1	-89.1	10.82
[1]1045	-63.6	-74.9	15.66				

[1]Melting point of $CaCl_2$.

TABLE 23. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Na_2O(s) + Cl_2(g) + C(s) = 2NaCl(s,\ell) + CO(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-123.3	-126.0	92.36	900	-121.8	-132.6	32.20
300	-123.2	-126.0	91.79	1000	-121.5	-133.8	29.24
400	-122.9	-126.9	69.33	[1]1073.8	-121.4	-134.7	27.42
500	-122.6	-128.0	55.95	1073.8	-107.9	-134.7	27.42
600	-122.4	-129.1	47.02	1100	-107.8	-135.3	26.88
700	-122.2	-130.2	40.65	1200	-107.9	-137.8	25.10
800	-122.0	-131.4	35.90	1300	-108.5	-140.3	23.59

[1]Melting point of NaCl.

TABLE 24. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$K_2O(s) + Cl_2(g) + C(s) = 2KCl(s,\ell) + CO(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-148.8	-151.5	111.05	900	-147.8	-157.8	38.32
300	-148.8	-151.5	110.37	1000	-147.4	-158.9	34.73
400	-148.5	-152.5	83.32	[1]1045	-147.2	-159.5	33.36
500	-148.3	-153.5	67.09	1045	-134.7	-159.5	33.36
600	-148.2	-154.5	56.28	1100	-134.4	-160.8	31.95
700	-148.1	-155.6	48.58	[2]1154	-134.0	-162.1	30.70
800	-147.9	-156.7	42.81				

[1]Melting point of KCl.
[2]Decomposition point of K_2O.

TABLE 25. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Al_2O_3(s) + 3Cl_2(g) + 3CO(g) = Al_2Cl_6(g) + 3CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-111.6	-111.6	∞	1000	-111.3	-65.5	14.32
100	-112.1	-107.4	234.72	1100	-111.2	-60.9	12.10
200	-112.0	-102.6	112.12	1200	-111.0	-56.3	10.25
298.15	-112.0	-98.0	71.84	1300	-110.9	-51.8	8.71
300	-112.0	-98.0	71.39	1400	-110.7	-47.2	7.37
400	-112.0	-93.3	50.98	1500	-110.6	-42.7	6.22
500	-111.9	-88.6	38.73	1600	-110.5	-38.2	5.22
600	-111.8	-83.9	30.56	1700	-110.4	-33.7	4.33
700	-111.7	-79.3	24.76	1800	-110.3	-29.2	3.55
800	-111.6	-74.7	20.41	1900	-110.2	-24.7	2.84
900	-111.5	-70.1	17.02	2000	-110.1	-20.1	2.20

TABLE 26. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Al_2O_3(s) + 3Cl_2(g) + 3CO(g) = 2AlCl_3(g) + 3CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-80.6	-80.6	∞	1000	-83.2	-69.4	15.17
100	-80.9	-80.0	174.84	1100	-83.5	-68.0	13.51
200	-80.9	-79.1	86.44	1200	-83.7	-66.6	12.13
298.15	-81.2	-78.1	57.25	1300	-84.0	-65.1	10.94
300	-81.2	-78.1	56.90	1400	-84.2	-63.7	9.94
400	-81.5	-77.1	42.13	1500	-84.5	-62.2	9.06
500	-81.9	-75.9	33.18	1600	-84.8	-60.7	8.29
600	-82.2	-74.7	27.21	1700	-85.1	-59.2	7.61
700	-82.5	-73.4	22.92	1800	-85.4	-57.6	6.99
800	-82.7	-72.1	19.70	1900	-85.7	-56.1	6.45
900	-83.0	-70.7	17.17	2000	-86.0	-54.5	5.96

TABLE 27. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$SiO_2(s) + 2Cl_2(g) + 2CO(g) = SiCl_4(g) + 2CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-74.6	-65.7	48.16	900	-75.1	-47.5	11.53
300	-74.6	-65.6	47.79	1000	-75.1	-44.4	9.70
400	-74.7	-62.6	34.20	1100	-75.0	-41.3	8.21
500	-74.7	-59.6	26.05	1200	-74.9	-38.3	6.98
600	-74.8	-56.6	20.62	1300	-74.8	-35.2	5.92
700	-74.8	-53.6	16.73	1400	-74.6	-32.2	5.03
800	-74.9	-50.5	13.80	1500	-74.5	-29.1	4.24
[1]847	-75.0	-49.1	12.67	1600	-74.3	-26.1	3.57
847	-75.2	-49.1	12.67	1700	-74.2	-23.1	2.97

[1]Transition point of SiO_2.

TABLE 28. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$TiO_2(s) + 2Cl_2(g) + 2CO(g) = TiCl_4(g) + 2CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-92.0	-84.2	61.72	1200	-92.8	-59.4	10.82
300	-92.0	-84.2	61.34	1300	-92.8	-56.6	9.52
400	-92.2	-81.5	44.53	1400	-92.7	-53.9	8.41
500	-92.4	-78.8	34.44	1500	-92.7	-51.1	7.45
600	-92.6	-76.1	27.72	1600	-92.7	-48.3	6.60
700	-92.7	-73.3	22.89	1700	-92.7	-45.5	5.85
800	-92.7	-70.5	19.26	1800	-92.8	-42.8	5.20
900	-92.8	-67.8	16.46	1900	-92.8	-40.0	4.60
1000	-92.8	-65.0	14.21	2000	-92.9	-37.2	4.07
1100	-92.8	-62.2	12.36				

TABLE 29. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Fe_2O_3(s) + 3Cl_2(g) + 3CO(g) = Fe_2Cl_6(g) + 3CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-162.3	-162.3	∞	[1]960	-166.1	-121.5	27.66
100	-162.5	-158.3	345.96	1000	-166.2	-119.6	26.14
200	-162.3	-154.2	168.50	1100	-166.4	-115.0	22.85
298.15	-162.4	-150.2	110.10	1200	-166.5	-110.3	20.09
300	-162.4	-150.1	109.35	1300	-166.7	-105.6	17.75
400	-162.7	-146.0	79.77	1400	-166.8	-100.9	15.75
500	-163.0	-141.8	61.98	1500	-166.9	-96.2	14.02
600	-163.4	-137.5	50.08	1600	-167.0	-91.5	12.50
700	-163.9	-133.2	41.59	1700	-167.1	-86.7	11.15
800	-164.5	-128.8	35.19	1800	-167.2	-82.0	9.96
900	-165.3	-124.2	30.16				

[1]Curie temperature of Fe_2O_3.

TABLE 30. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Fe_2O_3(s) + 3Cl_2(g) + 3CO(g) = 2FeCl_3(g) + 3CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-126.2	-126.2	∞	[1]960	-133.7	-119.2	27.14
100	-126.5	-126.4	276.25	1000	-133.9	-118.5	25.90
200	-126.8	-126.3	138.01	1100	-134.5	-117.0	23.25
298.15	-127.3	-125.9	92.29	1200	-135.1	-115.4	21.02
300	-127.3	-125.9	91.72	1300	-135.7	-113.7	19.11
400	-128.0	-125.3	68.46	1400	-136.2	-112.0	17.48
500	-128.8	-124.5	54.42	1500	-136.7	-110.2	16.06
600	-129.6	-123.6	45.02	1600	-137.2	-108.4	14.81
700	-130.5	-122.6	38.28	1700	-137.7	-106.6	13.70
800	-131.5	-121.4	33.16	1800	-138.1	-104.8	12.72
900	-132.7	-120.0	29.14				

[1]Curie temperature of Fe_2O_3.

TABLE 31. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$CaO(s) + Cl_2(g) + CO(g) = CaCl_2(s,\ell) + CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-106.0	-96.0	70.37	1045	-97.5	-71.9	15.04
300	-106.0	-96.0	69.94	1100	-97.1	-70.6	14.03
400	-105.9	-92.7	50.65	1200	-96.3	-68.2	12.42
500	-105.8	-89.4	39.08	1300	-95.5	-65.9	11.08
600	-105.6	-86.1	31.36	1400	-94.8	-63.7	9.94
700	-105.4	-82.9	25.88	1500	-94.0	-61.5	8.96
800	-105.1	-79.7	21.77	1600	-93.2	-59.4	8.11
900	-104.9	-76.5	18.58	1700	-92.5	-57.3	7.37
1000	-104.5	-73.3	16.02	1800	-91.8	-55.2	6.70
[1]1045	-104.3	-71.9	15.04				

[1]Melting point of $CaCl_2$.

TABLE 32. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Na_2O(s) + Cl_2(g) + CO(g) = 2NaCl(s,\ell) + CO_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-164.5	-154.6	113.32	900	-162.8	-135.7	32.95
300	-164.5	-154.6	112.63	1000	-162.3	-132.7	29.00
400	-164.3	-151.3	82.67	[1]1073.8	-162.0	-130.5	26.56
500	-164.1	-148.1	64.73	1073.8	-148.5	-130.5	26.56
600	-163.9	-144.9	52.78	1100	-148.4	-130.1	25.85
700	-163.6	-141.8	44.27	1200	-148.2	-128.4	23.38
800	-163.2	-138.7	37.89	1300	-148.6	-126.7	21.30

[1]Melting point of NaCl.

TABLE 33. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$K_2O(s) + Cl_2(g) + CO(g) = 2KCl(s,\ell) + CO_2(g)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-190.0	-180.2	132.09	900	-188.7	-160.9	39.07
300	-190.0	-180.1	131.20	1000	-188.2	-157.9	34.51
400	-189.9	-176.9	96.65	[1]1045	-187.9	-156.5	32.73
500	-189.8	-173.6	75.88	1045	-175.4	-156.5	32.73
600	-189.6	-170.4	62.07	1100	-174.9	-155.5	30.89
700	-189.4	-167.2	52.20	[2]1154	-174.4	-154.6	29.28
800	-189.1	-164.0	44.80				

[1]Melting point of KCl.
[2]Decomposition point of K_2O.

TABLE 34. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$[Al_2O_3(s) + 2SiO_2(s)] + 4NaCl(s,\ell) + Cl_2(g) + 0.5C(s) = Al_2Cl_6(g) + 2Na_2SiO_3(s,\ell) + 0.5CO_2(g)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	126.0	114.5	-83.93	[2]1073.8	122.0	86.7	-17.65
300	126.0	114.5	-83.41	1073.8	94.9	86.7	-17.65
400	125.8	110.6	-60.43	1100	94.7	86.5	-17.19
500	125.5	106.9	-46.73	1200	93.9	85.8	-15.63
600	125.2	103.2	-37.59	1300	93.3	85.2	-14.32
700	124.8	99.5	-31.07	[3]1362	93.0	84.8	-13.61
800	124.2	96.0	-26.23	1362	117.8	84.8	-13.61
[1]847	123.7	94.3	-24.33	1400	117.5	83.9	-13.10
847	123.4	94.3	-24.33	1500	116.7	81.5	-11.87
900	123.1	92.5	-22.46	1600	115.9	79.2	-10.82
1000	122.5	89.2	-19.49	1700	115.1	76.9	-9.89

[1]Transition point of SiO_2.
[2]Melting point of NaCl.
[3]Melting point of Na_2SiO_3.

TABLE 35. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$[Al_2O_3(s) + 2SiO_2(s)] + 4NaCl(s,\ell) + Cl_2(g) + 0.5C(s) = 2AlCl_3(g) + 2Na_2SiO_3(s,\ell) + 0.5CO_2(g)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	156.8	134.4	-98.52	[2]1073.8	149.8	80.5	-16.38
300	156.8	134.3	-97.84	1073.8	122.7	80.5	-16.38
400	156.2	126.9	-69.33	1100	122.4	79.4	-15.78
500	155.6	119.6	-52.28	1200	121.3	75.6	-13.77
600	154.9	112.5	-40.98	1300	120.3	71.8	-12.07
700	154.1	105.5	-32.94	[3]1362	119.7	69.5	-11.15
800	153.1	98.6	-26.94	1362	144.5	69.5	-11.15
[1]847	152.4	95.4	-24.62	1400	144.0	67.5	-10.54
847	152.1	95.4	-24.62	1500	142.9	62.0	-9.03
900	151.6	91.8	-22.29	1600	141.7	56.7	-7.74
1000	150.6	85.3	-18.64	1700	140.4	51.4	-6.61

[1]Transition point of SiO_2.
[2]Melting point of NaCl.
[3]Melting point of Na_2SiO_3.

TABLE 36. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$[Al_2O_3(s) + 2SiO_2(s)] + 4NaCl(s,\ell) + Cl_2(g) + C(s) = Al_2Cl_6(g) + 2Na_2SiO_3(s,\ell) + CO(g)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	146.6	128.9	-94.49	[2]1073.8	142.3	84.6	-17.22
300	146.6	128.8	-93.83	1073.8	115.2	84.6	-17.22
400	146.5	122.8	-67.09	1100	115.0	83.9	-16.67
500	146.3	116.9	-51.10	1200	114.1	81.1	-14.77
600	145.9	111.1	-40.47	1300	113.4	78.4	-13.18
700	145.5	105.3	-32.88	[3]1362	113.0	76.7	-12.31
800	144.8	99.6	-27.21	1362	137.7	76.7	-12.31
[1]847	144.3	97.0	-25.03	1400	137.4	75.0	-11.71
847	143.9	97.0	-25.03	1500	136.5	70.6	-10.29
900	143.6	94.1	-22.85	1600	135.5	66.3	-9.06
1000	142.9	88.6	-19.36	1700	134.5	62.0	-7.97

[1]Transition point of SiO_2.
[2]Melting point of NaCl.
[3]Melting point of Na_2SiO_3.

TABLE 37. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$[Al_2O_3(s) + 2SiO_2(s)] + 4NaCl(s,\ell) + Cl_2(g) + C(s) = 2AlCl_3(g) + 2Na_2SiO_3(s,\ell) + CO(g)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	177.4	148.8	-109.07	[2]1073.8	170.1	78.4	-15.96
300	177.4	148.6	-108.25	1073.8	143.0	78.4	-15.96
400	176.9	139.1	-76.00	1100	142.7	76.8	-15.26
500	176.3	129.6	-56.65	1200	141.4	70.9	-12.91
600	175.6	120.4	-43.86	1300	140.3	65.1	-10.94
700	174.8	111.2	-34.72	[3]1362	139.7	61.5	-9.87
800	173.7	102.2	-27.92	1362	164.4	61.5	-9.87
[1]847	173.0	98.1	-25.31	1400	163.9	58.6	-9.15
847	172.6	98.1	-25.31	1500	162.6	51.1	-7.45
900	172.1	93.4	-22.68	1600	161.3	43.8	-5.98
1000	171.0	84.7	-18.51	1700	159.9	36.5	-4.69

[1]Transition point of SiO_2.
[2]Melting point of NaCl.
[3]Melting point of Na_2SiO_3.

TABLE 38. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$[Al_2O_3(s) + 2SiO_2(s)] + 4NaCl(s,\ell) + Cl_2(g) + CO(g) = Al_2Cl_6(g) + 2Na_2SiO_3(s,\ell) + CO_2(g)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	105.4	100.2	-73.45	[2]1073.8	101.6	88.8	-18.07
300	105.4	100.1	-72.92	1073.8	74.6	88.8	-18.07
400	105.1	98.4	-53.76	1100	74.4	89.2	-17.72
500	104.8	96.8	-42.31	1200	73.8	90.5	-16.48
600	104.5	95.3	-34.71	1300	73.3	91.9	-15.45
700	104.1	93.8	-29.29	[3]1362	73.1	92.8	-14.89
800	103.6	92.3	-25.22	1362	97.9	92.8	-14.89
[1]847	103.2	91.7	-23.66	1400	97.6	92.7	-14.47
847	102.8	91.7	-23.66	1500	97.0	92.4	-13.46
900	102.6	91.0	-22.10	1600	96.3	92.1	-12.58
1000	102.1	89.7	-19.60	1700	95.6	91.8	-11.80

[1]Transition point of SiO_2.
[2]Melting point of NaCl.
[3]Melting point of Na_2SiO_3.

TABLE 39. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$[Al_2O_3(s) + 2SiO_2(s)] + 4NaCl(s,\ell) + Cl_2(g) + CO(g) = 2AlCl_3(g) + 2Na_2SiO_3(s,\ell) + CO_2(g)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	136.2	120.1	-88.04	[2]1073.8	129.5	82.6	-16.81
300	136.2	120.0	-87.42	1073.8	102.4	82.6	-16.81
400	135.5	114.7	-62.67	1100	102.1	82.1	-16.31
500	134.8	109.5	-47.86	1200	101.1	80.3	-14.62
600	134.2	104.5	-38.06	1300	100.3	78.6	-13.21
700	133.4	99.7	-31.13	[3]1362	99.8	77.6	-12.45
800	132.5	94.9	-25.93	1362	124.6	77.6	-12.45
[1]847	131.9	92.7	-23.92	1400	124.2	76.3	-11.91
847	131.5	92.7	-23.92	1500	123.1	72.9	-10.62
900	131.1	90.3	-21.93	1600	122.1	69.6	-9.51
1000	130.2	85.8	-18.75	1700	121.0	66.3	-8.52

[1]Transition point of SiO_2.
[2]Melting point of NaCl.
[3]Melting point of Na_2SiO_3.

TABLE 40. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$[Al_2O_3(s) + 2SiO_2(s)] + Na_2CO_3(s,\ell) + 2NaCl(s,\ell) + 2CaCl_2(s,\ell) = Al_2Cl_6(g) + 2Na_2CaSiO_4(s) + CO_2(g)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	284.5	257.4	-188.68	847	280.2	209.7	-54.11
300	284.5	257.2	-187.37	900	282.0	205.2	-49.83
400	283.9	248.2	-135.61	1000	281.9	196.7	-42.99
500	283.1	239.4	-104.64	[4]1045	277.3	192.9	-40.34
600	282.3	230.7	-84.03	1045	263.7	192.9	-40.34
700	281.6	222.2	-69.37	[5]1073.8	270.3	190.8	-38.83
[1]723	279.4	220.3	-66.59	1073.8	256.8	190.8	-38.83
723	279.2	220.3	-66.59	1100	253.8	189.2	-37.59
800	281.7	213.7	-58.38	[6]1123	251.2	187.9	-36.57
[2]830	281.9	211.2	-55.61	1123	244.1	187.9	-36.57
830	282.2	211.2	-55.61	1200	245.2	183.9	-33.49
[3]847	280.5	209.7	-54.11	1300	243.6	178.9	-30.08

[1]Transition point of Na_2CO_3.
[2]Transition point of Na_2CaSiO_4.
[3]Transition point of SiO_2.
[4]Melting point of $CaCl_2$.
[5]Melting point of NaCl.
[6]Melting point of Na_2CO_3.

TABLE 41. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$[Al_2O_3(s) + 2SiO_2(s)] + Na_2CO_3(s,\ell) + 2NaCl(s,\ell) + 2CaCl_2(s,\ell) = 2AlCl_3(g) + 2Na_2CaSiO_4(s) + CO_2(g)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	315.3	277.3	-203.27	847	308.9	210.8	-54.39
300	315.3	277.1	-201.87	900	310.5	204.5	-49.66
400	314.3	264.4	-144.46	1000	310.0	192.8	-42.14
500	313.1	252.1	-110.19	[4]1045	305.2	187.6	-39.23
600	312.0	240.0	-87.42	1045	291.6	187.6	-39.23
700	310.9	228.1	-71.22	[5]1073.8	298.1	184.5	-37.55
[1]723	308.6	225.4	-68.13	1073.8	284.6	184.5	-37.55
723	308.4	225.4	-68.13	1100	281.5	182.1	-36.18
800	310.6	216.3	-59.09	[6]1123	278.8	180.1	-35.05
[2]830	310.7	212.8	-56.03	1123	271.7	180.1	-35.05
830	311.0	212.8	-56.03	1200	272.5	173.7	-31.64
[3]847	309.2	210.8	-54.39	1300	270.5	165.5	-27.82

[1]Transition point of Na_2CO_3.
[2]Transition point of Na_2CaSiO_4.
[3]Transition point of SiO_2.
[4]Melting point of $CaCl_2$.
[5]Melting point of NaCl.
[6]Melting point of Na_2CO_3.

TABLE 42. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$$[Al_2O_3(s) + 2SiO_2(s)] + 4NaCl(s,\ell) + CaCl_2(s,\ell) + CaO(s) = Al_2Cl_6(g) + 2Na_2CaSiO_4(s)$$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	266.4	250.2	-183.40	847	264.8	221.4	-57.13
300	266.4	250.1	-182.20	900	266.8	218.5	-53.06
400	265.9	244.7	-133.70	1000	267.3	213.1	-46.57
500	265.4	239.5	-104.69	[3]1045	262.9	210.8	-44.09
600	265.3	234.3	-85.34	1045	256.1	210.8	-44.09
700	265.6	229.1	-71.53	[4]1073.8	263.0	209.3	-42.60
800	266.3	223.9	-61.17	1073.8	236.0	209.3	-42.60
[1]830	266.5	222.3	-58.53	1100	233.3	208.7	-41.46
830	266.9	222.3	-58.53	1200	232.8	206.5	-37.61
[2]847	265.2	221.4	-57.13	1300	232.2	204.4	-34.36

[1]Transition point of Na_2CaSiO_4.
[2]Transition point of SiO_2.
[3]Melting point of $CaCl_2$.
[4]Melting point of NaCl.

TABLE 43. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$[Al_2O_3(s) + 2SiO_2(s)] + 4NaCl(s,\ell) + CaCl_2(s,\ell) + CaO(s) = 2AlCl_3(g) + 2Na_2CaSiO_4(s)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	297.2	270.1	-197.99	847	293.6	222.4	-57.39
300	297.2	269.9	-196.62	900	295.3	217.8	-52.89
400	296.4	260.9	-142.55	1000	295.4	209.2	-45.72
500	295.5	252.2	-110.24	[3]1045	290.8	205.5	-42.98
600	295.0	243.6	-88.73	1045	284.0	205.5	-42.98
700	294.8	235.0	-73.37	[4]1073.8	290.8	203.1	-41.34
800	295.2	226.5	-61.88	1073.8	263.8	203.1	-41.34
[1]830	295.3	223.9	-58.96	1100	261.0	201.6	-40.05
830	295.6	223.9	-58.96	1200	260.1	196.3	-35.75
[2]847	293.9	222.4	-57.39	1300	259.2	191.0	-32.11

[1]Transition point of Na_2CaSiO_4.
[2]Transition point of SiO_2.
[3]Melting point of $CaCl_2$.
[4]Melting point of NaCl.

TABLE 44. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$AlCl_3(g) = 0.5\,Al_2Cl_6(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-15.5	-15.5	∞	1000	-14.1	1.9	-0.42
100	-15.6	-13.7	29.94	1100	-13.9	3.5	-.70
200	-15.5	-11.8	12.89	1200	-13.7	5.1	-.93
298.15	-15.4	-9.9	7.26	1300	-13.5	6.7	-1.13
300	-15.4	-9.9	7.21	1400	-13.3	8.2	-1.28
400	-15.2	-8.1	4.43	1500	-13.1	9.7	-1.41
500	-15.0	-6.4	2.80	1600	-12.9	11.3	-1.54
600	-14.8	-4.6	1.68	1700	-12.7	12.8	-1.65
700	-14.6	-3.0	.94	1800	-12.5	14.2	-1.72
800	-14.4	-1.3	.36	1900	-12.3	15.7	-1.81
900	-14.3	.3	-.07	2000	-12.1	17.2	-1.88

TABLE 45. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction $AlCl_3(s,\ell) = 0.5Al_2Cl_6(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	13.5	13.5	∞	600	3.2	-2.0	0.73
100	13.9	10.6	-23.17	700	2.3	-2.8	.87
200	13.8	7.4	-8.09	800	1.4	-3.4	.93
298.15	13.5	4.3	-3.15	900	.6	-4.0	.97
300	13.5	4.3	-3.13	1000	-.3	-4.4	.96
400	13.2	1.3	-.71	1100	-1.1	-4.8	.95
[1]442.85	13.0	.0	.00	1200	-2.0	-5.1	.93
[2]465.7	12.9	-.7	.33	1300	-2.8	-5.3	.89
465.7	4.4	-.7	.33	1400	-3.7	-5.5	.86
500	4.1	-1.0	.44	1500	-4.5	-5.6	.82

[1]Al_2Cl_6 vapor pressure = 1 atm.
[2]Melting point of $AlCl_3$.

TABLE 46. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction $AlCl_3(s,\ell) = AlCl_3(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	29.0	29.0	∞	700	16.9	0.2	- 0.06
100	29.5	24.3	-53.11	[2]708.35	16.8	.0	.00
200	29.3	19.2	-20.98	800	15.9	-2.1	.57
298.15	28.9	14.3	-10.48	900	14.8	-4.3	1.04
300	28.9	14.2	-10.34	1000	13.8	-6.4	1.40
400	28.4	9.4	-5.14	1100	12.7	-8.3	1.65
[1]465.7	28.0	6.3	-2.96	1200	11.7	-10.2	1.86
465.7	19.5	6.3	-2.96	1300	10.6	-12.0	2.02
500	19.1	5.3	-2.32	1400	9.6	-13.7	2.14
600	18.0	2.7	-.98	1500	8.6	-15.3	2.23

[1]Melting point of $AlCl_3$.
[2]$AlCl_3$ vapor pressure = 1 atm.

TABLE 47. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction $FeCl_3(g) = 0.5Fe_2Cl_6(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-18.0	-18.0	∞	1000	-16.1	-0.5	0.11
100	-18.0	-15.9	34.75	1100	-15.9	1.0	-.20
200	-17.8	-14.0	15.30	1200	-15.7	2.5	-.46
298.15	-17.6	-12.2	8.94	1300	-15.5	4.0	-.67
300	-17.5	-12.1	8.81	1400	-15.3	5.5	-.86
400	-17.3	-10.4	5.68	1500	-15.1	7.0	-1.02
500	-17.1	-8.6	3.76	1600	-14.9	8.5	-1.16
600	-16.9	-7.0	2.55	1700	-14.7	9.9	-1.27
700	-16.7	-5.3	1.65	1800	-14.5	11.4	-1.38
800	-16.5	-3.7	1.01	1900	-14.3	12.8	-1.47
900	-16.3	-2.1	.51	2000	-14.1	14.2	-1.55

TABLE 48. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction $FeCl_3(s,\ell) = 0.5Fe_2Cl_6(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	17.0	17.0	∞	400	16.8	5.7	-3.11
100	17.3	14.4	-31.47	500	16.3	3.0	-1.31
200	17.3	11.4	-12.46	[1]577	15.8	.9	-.34
298.15	17.2	8.6	-6.30	577	5.6	.9	-.34
300	17.2	8.5	-6.19	600	5.3	.7	-.25
				700	4.3	.1	-.03

[1]Melting point of $FeCl_3$.

TABLE 49. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction $FeCl_3(s,\ell) = FeCl_3(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	35.0	35.0	∞	400	34.1	16.0	-8.74
100	35.3	30.3	-66.22	500	33.4	11.6	-5.07
200	35.1	25.4	-27.76	[1]577	32.8	8.3	-3.14
298.15	34.7	20.7	-15.17	577	22.5	8.3	-3.14
300	34.7	20.6	-15.01	600	22.2	7.7	-2.80
				700	21.0	5.4	-1.69

[1] Melting point of $FeCl_3$.

TABLE 50. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction $FeCl_3(g) = FeCl_2(g) + 0.5Cl_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	26.8	26.8	∞	1000	26.6	11.4	-2.49
100	27.1	25.5	-55.73	1100	26.6	9.9	-1.97
200	27.1	23.8	-26.01	1200	26.6	8.4	-1.53
298.15	27.0	22.3	-16.35	1300	26.5	6.9	-1.16
300	27.0	22.2	-16.17	1400	26.5	5.4	-.84
400	26.9	20.6	-11.26	1500	26.5	3.9	-.57
500	26.9	19.1	-8.35	1600	26.5	2.3	-.31
600	26.8	17.5	-6.37	1700	26.6	.8	-.10
700	26.7	16.0	-5.00	1800	26.6	-.7	.08
800	26.7	14.5	-3.96	1900	26.6	-2.2	.25
900	26.6	12.9	-3.13	2000	26.7	-3.7	.40

TABLE 51. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction $FeCl_2(s,\ell) = FeCl_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	48.5	48.5	∞	700	46.0	18.6	-5.81
100	48.8	44.0	-96.16	800	45.4	14.8	-4.04
200	48.4	39.4	-43.05	900	44.8	11.0	-2.67
298.15	48.0	35.1	-25.73	[1]950	44.5	9.1	-2.09
300	48.0	35.0	-25.50	950	34.3	9.1	-2.09
400	47.5	30.7	-16.77	1000	33.8	7.8	-1.70
500	47.0	26.6	-11.63	1100	32.8	5.2	-1.03
600	46.5	22.6	-8.23	1200	31.9	2.8	-.51

[1]Melting point of $FeCl_2$.

TABLE 52. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction $TiCl_4(\ell) = TiCl_4(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	9.9	2.5	-1.83	[1]410	8.35	0	0
325	9.5	1.9	-1.28	425	8.15	-.3	.15
350	9.2	1.3	-.81	450	7.8	-.8	.39
375	8.85	.75	-.44	475	7.5	-1.25	.58
400	8.5	.2	-.11	500	7.15	-1.7	.74

[1]Boiling point of $TiCl_4$.

TABLE 53. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$3SiCl_4(g) + 2Al_2O_3(s) = 2Al_2Cl_6(g) + 3SiO_2(s)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-0.3	1.0	-0.73	900	2.5	2.2	-0.53
300	-.3	1.0	-.73	1000	2.6	2.2	-.48
400	.1	1.4	-.76	1100	2.6	2.1	-.42
500	.4	1.7	-.74	1200	2.6	2.1	-.38
600	.6	1.9	-.69	1300	2.5	2.1	-.35
700	.9	2.1	-.66	1400	2.4	2.0	-.31
800	1.4	2.2	-.60	1500	2.2	2.0	-.29
[1]847	1.9	2.2	-.57	1600	2.0	2.0	-.27
847	2.4	2.2	-.57	1700	1.7	2.0	-.26

[1]Transition point of SiO_2.

TABLE 54. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$3SiCl_4(g) + 2Al_2O_3(s) = 4AlCl_3(g) + 3SiO_2(s)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	61.3	40.8	-29.91	900	59.5	0.9	-0.22
300	61.3	40.7	-29.65	1000	58.8	-5.6	1.22
400	61.0	33.8	-18.47	1100	58.1	-12.0	2.38
500	60.5	27.1	-11.85	1200	57.3	-18.3	3.33
600	60.0	20.4	-7.43	1300	56.4	-24.6	4.14
700	59.5	13.9	-4.34	1400	55.4	-30.8	4.81
800	59.2	7.4	-2.02	1500	54.5	-36.9	5.38
[1]847	59.3	4.3	-1.11	1600	53.5	-43.0	5.87
847	59.8	4.3	-1.11	1700	52.4	-49.0	6.30

[1]Transition point of SiO_2.

TABLE 55. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$SiCl_4(g) + O_2(g) = SiO_2(s) + 2Cl_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K	T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-60.7	-57.3	42.00	900	-60.1	-50.2	12.19
300	-60.7	-57.2	41.67	1000	-60.0	-49.1	10.73
400	-60.8	-56.1	30.65	1100	-59.9	-48.1	9.56
500	-60.8	-54.9	24.00	1200	-59.8	-47.0	8.56
600	-60.8	-53.7	19.56	1300	-59.7	-45.9	7.72
700	-60.7	-52.5	16.39	1400	-59.6	-44.9	7.01
800	-60.5	-51.3	14.01	1500	-59.6	-43.8	6.38
[1]847	-60.3	-50.8	13.11	1600	-59.5	-42.8	5.85
847	-60.2	-50.8	13.11	1700	-59.4	-41.7	5.36

[1]Transition point of SiO_2.

TABLE 56. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$2AlCl_3(g) + 1.5O_2(g) = Al_2O_3(s) + 3Cl_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-119.646	-119.646	∞
100	-120.433	-116.060	253.646
200	-121.326	-111.303	121.624
298.15	-121.700	-106.285	77.908
300	-121.703	-106.189	77.358
400	-121.710	-101.008	55.187
500	-121.513	-95.853	41.897
600	-121.199	-90.751	33.056
700	-120.814	-85.704	26.758
800	-120.383	-80.718	22.051
900	-119.918	-75.788	18.404
1000	-119.422	-70.908	15.497
1100	-118.902	-66.082	13.129
1200	-118.354	-61.303	11.165
1300	-117.782	-56.573	9.511
1400	-117.187	-51.888	8.100
1500	-116.570	-47.243	6.883
1600	-115.934	-42.642	5.825
1700	-115.281	-38.086	4.896
1800	-114.612	-33.558	4.074
1900	-113.935	-29.082	3.345
2000	-113.242	-24.632	2.692

TABLE 57. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Al_2Cl_6(g) + 1.5O_2(g) = Al_2O_3(s) + 3Cl_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-88.681	-88.681	-
100	-89.199	-88.689	193.828
200	-90.230	-87.763	95.902
298.15	-90.900	-86.394	63.327
300	-90.909	-86.365	62.916
400	-91.271	-84.787	46.325
500	-91.451	-83.145	36.342
600	-91.520	-81.476	29.677
700	-91.525	-79.800	24.914
800	-91.483	-78.127	21.343
900	-91.413	-76.465	18.568
1000	-91.310	-74.806	16.349
1100	-91.184	-73.161	14.536
1200	-91.031	-71.528	13.027
1300	-90.854	-69.910	11.753
1400	-90.654	-68.307	10.663
1500	-90.434	-66.718	9.721
1600	-90.193	-65.144	8.898
1700	-89.937	-63.590	8.175
1800	-89.665	-62.044	7.533
1900	-89.384	-60.524	6.962
2000	-89.087	-59.011	6.448

TABLE 58. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$2FeCl_2(s,\ell) + 1.5O_2(g) = Fe_2O_3(s) + 2Cl_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-30.816	-30.816	-
100	-31.441	-32.470	70.962
200	-32.785	-32.978	36.036
298.15	-33.600	-32.879	24.101
300	-33.611	-32.874	23.948
400	-34.041	-32.558	17.788
500	-34.263	-32.158	14.056
600	-34.352	-31.727	11.557
700	-34.337	-31.287	9.768
800	-34.193	-30.865	8.432
900	-33.835	-30.466	7.398
[1]950	-33.456	-30.284	6.967
950	-54.016	-30.284	6.967
1000	-54.355	-29.028	6.344
1100	-55.298	-26.452	5.256
1200	-56.250	-23.787	4.332

[1]Melting point of $FeCl_2$.

TABLE 59. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$2FeCl_2(g) + 1.5\,O_2(g) = Fe_2O_3(s) + 2Cl_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-127.770	-127.770	∞
100	-128.977	-120.556	263.472
200	-129.639	-111.815	122.184
298.15	-129.600	-103.052	75.538
300	-129.594	-102.885	74.950
400	-129.085	-94.053	51.387
500	-128.317	-85.379	37.319
600	-127.369	-76.877	28.002
700	-126.278	-68.547	21.401
800	-125.014	-60.386	16.496
900	-123.503	-52.395	12.723
960	-122.310	-47.687	10.856
960	-122.310	-47.687	10.856
1000	-121.921	-44.586	9.744
1100	-120.967	-36.902	7.332
1200	-120.042	-29.297	5.336
1300	-119.141	-21.767	3.659
1400	-118.268	-14.307	2.233
1500	-117.420	-6.915	1.008
1600	-116.597	.418	- .057
1700	-115.798	7.709	- .991
1800	-115.021	14.962	-1.817

TABLE 60. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$2FeCl_3(s,\ell) + 1.5O_2(g) = Fe_2O_3(s) + 3Cl_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-4.056	-4.056	∞
100	-4.120	-8.938	19.533
200	-5.260	-13.321	14.556
298.15	-6.160	-17.070	12.513
300	-6.174	-17.138	12.485
350	-6.448	-18.940	11.826
350	-6.544	-18.940	11.826
400	-6.962	-20.682	11.300
500	-7.733	-24.025	10.501
[1]577	-8.345	-26.489	10.033
577	-28.939	-26.489	10.033
600	-29.311	-26.385	9.610
700	-30.815	-25.774	8.047

[1]Melting point of $FeCl_3$.

TABLE 61. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$2FeCl_3(g) + 1.5O_2(g) = Fe_2O_3(s) + 3Cl_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-74.082	-74.082	∞
100	-74.803	-69.629	152.172
200	-75.492	-64.149	70.098
298.15	-75.600	-58.536	42.907
300	-75.596	-58.428	42.564
400	-75.232	-52.754	28.823
500	-74.595	-47.204	20.632
600	-73.768	-41.800	15.226
700	-72.787	-36.546	11.410
800	-71.625	-31.449	8.591
900	-70.206	-26.509	6.437
960	-69.062	-23.627	5.379
960	-69.062	-23.627	5.379
1000	-68.704	-21.741	4.751
1100	-67.817	-17.092	3.396
1200	-66.940	-12.515	2.279
1300	-66.071	-8.009	1.346
1400	-65.213	-3.575	.558
1500	-64.360	.795	-.116
1600	-63.513	5.104	-.697
1700	-62.671	9.368	-1.204
1800	-61.835	13.596	-1.651

TABLE 62. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$Fe_2Cl_6(g) + 1.5O_2(g) = Fe_2O_3(s) + 3Cl_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K
0	-38.021	-38.021	∞
100	-38.786	-37.736	82.470
200	-39.951	-36.195	39.551
298.15	-40.500	-34.210	25.076
300	-40.505	-34.169	24.892
400	-40.568	-32.040	17.506
500	-40.348	-29.930	13.082
600	-39.932	-27.882	10.156
700	-39.358	-25.916	8.091
800	-38.602	-24.048	6.569
900	-37.584	-22.285	5.411
960	-36.682	-21.289	4.847
960	-36.682	-21.289	4.847
1000	-36.485	-20.652	4.513
1100	-36.000	-19.096	3.794
1200	-35.523	-17.577	3.201
1300	-35.055	-16.096	2.706
1400	-34.595	-14.650	2.287
1500	-34.142	-13.246	1.930
1600	-33.694	-11.874	1.622
1700	-33.252	-10.523	1.353
1800	-32.815	-9.188	1.116

TABLE 63. - Enthalpy, Gibbs energy, and logarithm of the equilibrium constant of the reaction

$TiCl_4(g) + O_2(g) = TiO_2(s) + 2Cl_2(g)$

T, K	ΔH°, kcal	ΔG°, kcal	Log K
298.15	-43.270	-38.745	28.400
300	-43.271	-38.716	28.205
400	-43.261	-37.196	20.323
500	-43.169	-35.690	15.600
600	-43.021	-34.208	12.460
700	-42.845	-32.752	10.225
800	-42.657	-31.323	8.557
900	-42.469	-29.917	7.265
1000	-42.285	-28.531	6.235
1100	-42.103	-27.164	5.397
1200	-41.920	-25.814	4.701
1300	-41.731	-24.480	4.115
1400	-41.531	-23.160	3.615
1500	-41.315	-21.855	3.184
1600	-41.082	-20.567	2.809
1700	-40.831	-19.295	2.481
1800	-40.561	-18.032	2.189
1900	-40.274	-16.792	1.931
2000	-39.961	-15.563	1.701

TABLE 64. - Gibbs energy comparison for carbon reduction chlorination of oxides; basis is one gram atom of oxygen of each oxide

$$^{1}M_xO(s) + Cl_2(g) + 0.5C(s) = M_xCl_2 + 0.5CO_2(g)$$

T, K	ΔG°, kcal						
	$(1/3)Al_2O_3$	$0.5SiO_2$	$0.5TiO_2$	$(1/3)Fe_2O_3$	CaO	Na_2O	K_2O
298	-18.3	-18.5	-27.8	-35.7	-81.7	-140.3	-165.8
300	-18.3	-18.5	-27.8	-35.7	-81.7	-140.3	-165.8
400	-18.9	-19.1	-28.6	-36.5	-80.5	-139.1	-164.7
500	-19.5	-19.8	-29.4	-37.2	-79.3	-138.0	-163.6
600	-20.1	-20.4	-30.1	-37.9	-78.2	-137.0	-162.5
700	-20.6	-21.0	-30.9	-38.6	-77.1	-136.0	-161.4
800	-21.2	-21.6	-31.6	-39.3	-76.0	-135.0	-160.4
900	-22.0	-22.2	-32.3	-39.9	-74.9	-134.1	-159.4
1000	-23.7	-22.7	-33.0	-40.4	-73.9	-133.2	-158.4
1100	-25.3	-23.3	-33.7	-41.8	-73.2	-132.7	-158.1
1200	-26.9	-23.8	-34.4	-43.2	-73.0	-133.1	
1300	-28.5	-24.4	-35.1	-44.7	-72.7	-133.5	
1400	-30.1	-24.9	-35.8	-46.2	-72.5		
1500	-31.6	-25.5	-36.4	-47.6	-72.4		
1600	-33.1	-26.0	-37.1	-49.1	-72.3		
1700	-34.7	-26.5	-37.7	-50.5	-72.2		

[1] M = Al, Si, Ti, Fe, Ca, Na, and K.

x = metal subscript divided by oxygen subscript in oxide formula.

DISCUSSION

Available thermodynamic data show that in the absence of other, possibly unknown, factors, carbon reduction and chlorination of clay would yield aluminum chloride as monomeric and dimeric vapor. The overall process can be represented by reactions 1-2. Reaction 1, forming Al_2Cl_6, is the predominant reaction below 880 K, and reaction 2, yielding $AlCl_3$, is predominant above this temperature. The process also can be represented as consisting of two steps, with oxidation of carbon to CO (reactions 3-4) and with oxidation of CO to CO_2 (reactions 5-6). Standard Gibbs energy changes (tables 1-6) for all six reactions are highly negative, and if equilibrium were attainable, the reactions would go practically to completion. Comparative standard Gibbs energies indicate that formation of CO_2 will predominate below 970 K and that formation of CO will predominate above this temperature. Below 970 K, CO reduction is more favorable than carbon reduction. Examination of chlorination enthalpies shows the carbon-to-CO step (tables 3-4) to be endothermic, while the CO-to-CO_2 step (tables 5-6) is highly exothermic, resulting in an overall exothermic process (tables 1-2).

Thermodynamic calculations for reactions 7-33 provide information on the relative equilibrium conversion in the reduction-chlorination of the individual constituents and associated substances found in clay (α-Al_2O_3, SiO_2, and oxides of Fe, Ti, Ca, Na, and K). These chlorination reactions also are given with conversion of carbon to CO_2 (reactions 7-15) and as separate steps, carbon to CO (reactions 16-24) and CO to CO_2 (reactions 25-33). Standard Gibbs energy changes (tables 7-33) show that if equilibrium is reached, these reactions would proceed virtually to completion. The general conclusions given in the preceding paragraph, on Al_2Cl_6 versus $AlCl_3$ formation and on CO_2 versus CO formation, apply here also. It is indicated that, with the exception of SiO_2, all the other oxides should be chlorinated, at all temperatures, more completely than Al_2O_3. The standard Gibbs energy change for chlorination of Al_2O_3 becomes more negative than for the chlorination of SiO_2 above 915 K. Table 64 compares standard Gibbs energy changes per oxygen equivalent for reactions 7-15.

The highly positive standard Gibbs energy changes for reactions 34-43 (tables 34-43) imply that the various additives, NaCl, Na_2CO_3, $CaCl_2$, and CaO, do not promote the formation of silicates to decrease the formation of $SiCl_4$.

Available standard Gibbs energy values for the aluminum chloride vapor equilibrium (table 44) predict that the vapor should be predominantly dimeric below 880 K and monomeric above this temperature. Data on the vaporization of aluminum chloride (tables 45-46) show that the dimeric vapor pressure should reach 1 atm at 443 K and that the monomeric pressure should reach 1 atm at 708 K.

Table 48 provides data on the vaporization of $FeCl_3$ to the dimeric vapor. Interpolation of the data in this table at 443 K (the boiling point of $AlCl_3$) leads to an Fe_2Cl_6 vapor pressure of 3.6×10^{-5} atm. Extrapolation of the data yields a boiling temperature of 715 K for $FeCl_3$. Values in table 49, on the vaporization of $FeCl_3$ to the monomer, show the monomeric pressure to be lower than the dimeric pressure at all temperatures listed. Calculations for the ferric chloride vapor equilibrium (table 47) indicate that, up to 1,000 K, dimer formation should predominate.

Standard Gibbs energy changes in table 50 show that $FeCl_3$ is stable with respect to decomposition into $FeCl_2$ and Cl_2 until nearly 1,800 K. Table 51 pro-

vides vaporization data for the dichloride. Extrapolation of the data in table 51 yields 1,300 K as the boiling point of $FeCl_2$.

Results of the calculations for reactions 44-51 indicate that iron chlorides can be effectively separated from $AlCl_3$ by subliming the aluminum compound around 443 K. Less than 0.004 mole-pct Fe should be left in the $AlCl_3$; however, any mixed chloride compounds or solution formation could alter this figure.

Table 52 provides vaporization data for $TiCl_4$. The boiling point of the liquid is 410 K. At this temperature, the vapor pressure of Al_2Cl_6 is 0.3 atm.

According to the calculations in table 54, recycling of the $SiCl_4$ vapor to react with clay to form $AlCl_3$ (reactions 53-54) is thermodynamically possible above 915 K. Standard Gibbs energy changes in table 55 for recovery of Cl_2 from $SiCl_4$ vapor by means of O_2 are negative at all listed temperatures. Data in tables 57-63 on oxidation of Al, Fe, and Ti chlorides also show negative Gibbs energy changes.

The above considerations of equilibrium conditions have shown that chlorination of clay in the presence of carbon or CO is thermodynamically feasible over a wide range of temperature. Chlorination above 915 K should greatly reduce the ratio of $SiCl_4$ to $AlCl_3$ formed. Reduction by CO is thermodynamically preferable to reduction by carbon below 970 K. After chlorination, the chlorides of Na, K, and Ca will be in the condensed phase. A possible method of separation of $SiCl_4$ from the aluminum chloride vapor is recycling the vapor over fresh clay above 915 K. The SiO_2 formed on the surface of the clay particles by this procedure may interfere with further chlorination, and it may be preferable to separate the aluminum and silicon chlorides by fractional distillation. Separation of $AlCl_3$ from iron chloride may be possible by sublimination of $AlCl_3$ near 443 K. Avramenko (1) obtained $AlCl_3$ containing less than 1 ppm Fe by means of a multiple vacuum zone sublimation method; however, he did not report the yield of product. Fractional distillation to remove $TiCl_4$ also may be possible.

In the practical application of conclusions based on thermodynamic considerations, it should be kept in mind that reaction rates, transport, and other factors may exist to hinder a reaction that is thermodynamically favorable, and equilibrium may not be attainable. Other chemical reactions involving unknown gas, liquid, and solid species are also possible. Evaluation of reaction rate factors in the chlorination of clay will be the subject of another publication.

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